Office of Technical Assistance Research Proposal

Investigation of the Hydrogen Bonding Solubility Parameter

BACKGROUND

Substances that are defined as HAPs (Hazardous Air Pollutants), VOCs (Volatile Organic Compounds), or ODSs (Ozone Depleting Substances), many of which are reportable under TURA, find extensive use as solvents for various linear polymers such as inks, paints, coatings, etc. at numerous industries in Massachusetts. Acetone, MEK and toluene are three such solvents. For example, in the manufacturing of coated and laminated paper (SIC codes 2671 and 2672), 4.3 million lbs. of acetone, 3 million lbs. of MEK, and 5 million lbs. of toluene were reported under TURA in 1998 by such companies as Rexam Image Products, Madico, and Ideal Tape. Also in 1998, manufacturers of paints and coatings (SIC code 2851) such as Savogran, Sterling Clark Lurton, Franklin Paint Co., Camger Chemical Systems, and Surface Coatings, Inc. reported the use of 1.4 million lbs. of acetone, 1 million lbs. of MEK, and 5 million lbs. of toluene. It is felt that improvements in the ability to evaluate solubility parameters would facilitate the more efficient use of TURA-regulated solvents in a variety of industrial processes, thereby reducing the use of these chemicals.

Solubility parameters of the Hansen type are used for determining the solubility of one compound in another. The overall solubility parameter is made up of contributions from the different intermolecular attractions - dispersion, dipole, or hydrogen bonding. The hydrogen bonding parameter is the most troublesome in that it does not seem to fit into the Hansen formalism. The usual theoretical prediction of solubility is that based on the Gibb's Free Energy equation:

$$\Delta G = \Delta H - T\Delta S.$$

Here ΔG is the change in Gibb's Free Energy, it is negative for solution to be realized. ΔH is the change in enthalpy, and ΔS the change in entropy. In the usual treatment, the solubility parameter shows up in the enthalpy term while the entropy change is neglected. However, there is an increasing awareness that there are entropy contributions associated with the molecular attractions that may be important. In a recent paper by Schneider (1), evidence is offered that entropic contributions occur with these attractions that are not characterized by the solubility parameter.

It is the writer's belief that by use of microcalorimetry, heats of solution can be measured and compared to solubility parameter predictions. This would contribute to a more accurate understanding of solubility parameters, and particularly the hydrogen bonding parameter.

Hydrogen bonding is also operative in many biological processes. The DNA molecule holds its helical shape by hydrogen bonding. A successful outcome of this work may have a significant impact on the biotechnology and pharmaceutical industries in Massachusetts. A recent report by Sharma (2) describes the rapid growth of these industries in Massachusetts. Data from 1992 shows that nearly $0.5 billion in pharmaceuticals were shipped from Massachusetts.

SCOPE OF PROBLEM

Improving the predictability of solution in the case of the hydrogen bond and possibly other attractions as well would be of benefit in the industry sectors mentioned above and possibly other sectors.

OBJECTIVE

The objective of this work is to improve the predictability of solubility of one compound in the other and to gain a clearer insight into the solution process.

OTA can assist in the identification of an industry partner.

SCOPE OF WORK

A microcalorimeter needs to be obtained and precise measurements made on heats of solution.

(1) H.A. Schneider, J. Res. Nat. Inst. Of Standards and Technology, p229,V.102

(2) A. Sharma, University of Massachusetts at Amherst, “Economic Impact of the Pharmaceutical Industry on Massachusetts”. Available through the Donahue Institute.